CHAPTER III

THEORY

The success of any simulation study depends on the appropriateness of its mathematic model. This chapter presents a brief discussion of the basic theory of aerosol filtration, and the basic principle of the stochastic model and the present simplified model.

3.1 Basic theory of aerosol depostion on a filter fiber

3.1.1 Kuwabara flow field

Kuwabara (1959) solved the Navier-Stokes equations for viscous flow. Figure 3.1 shows the flow cells in a fibrous filter consisting of parallel fibers, spaced randomly and transverse to the flow. The mean flow is directed from left to right with a velocity equal to U. The vorticity would be negative on the upper side of a cylinder and positive on the lower side of a cylinder. An ideal cell for the mathematical model is shown in Figure 3.2, Kuwabara considered that each cylinder of radius R_f is enclosed by an imaginary cylindrical cell of radius R_c. If there are n parallel fibers per unit volume of filter, the volume fraction or packing density α is

$$\alpha = n \pi R_f^2 \tag{3.1}$$

and Rc is adjusted so that

$$n \pi R_c^2 = 1 \tag{3.2}$$

Thus
$$R_c = \frac{R_f}{\sqrt{\alpha}} \tag{3.3}$$

The boundary conditions used by Kuwabara were that velocity is zero on the surface of fiber and on the surface of the cell. The stream function, ψ, and the velocity component, U_x,U_y and U_z, expressed in dimensionless form are

$$\psi = \frac{Y}{2K}\left[(1-\frac{\alpha}{2})\frac{1}{X^2+Y^2} - (1-\alpha) + \ln(X^2+Y^2) - \frac{\alpha}{2}(X^2+Y^2)\right] \tag{3.4}$$

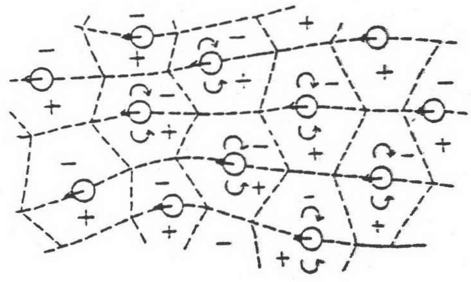

Figure 3.1a Vorticity around cylinder

(the broken lines are zero vorticity)

Figure 3.1b Mean flow velocity around cylinder

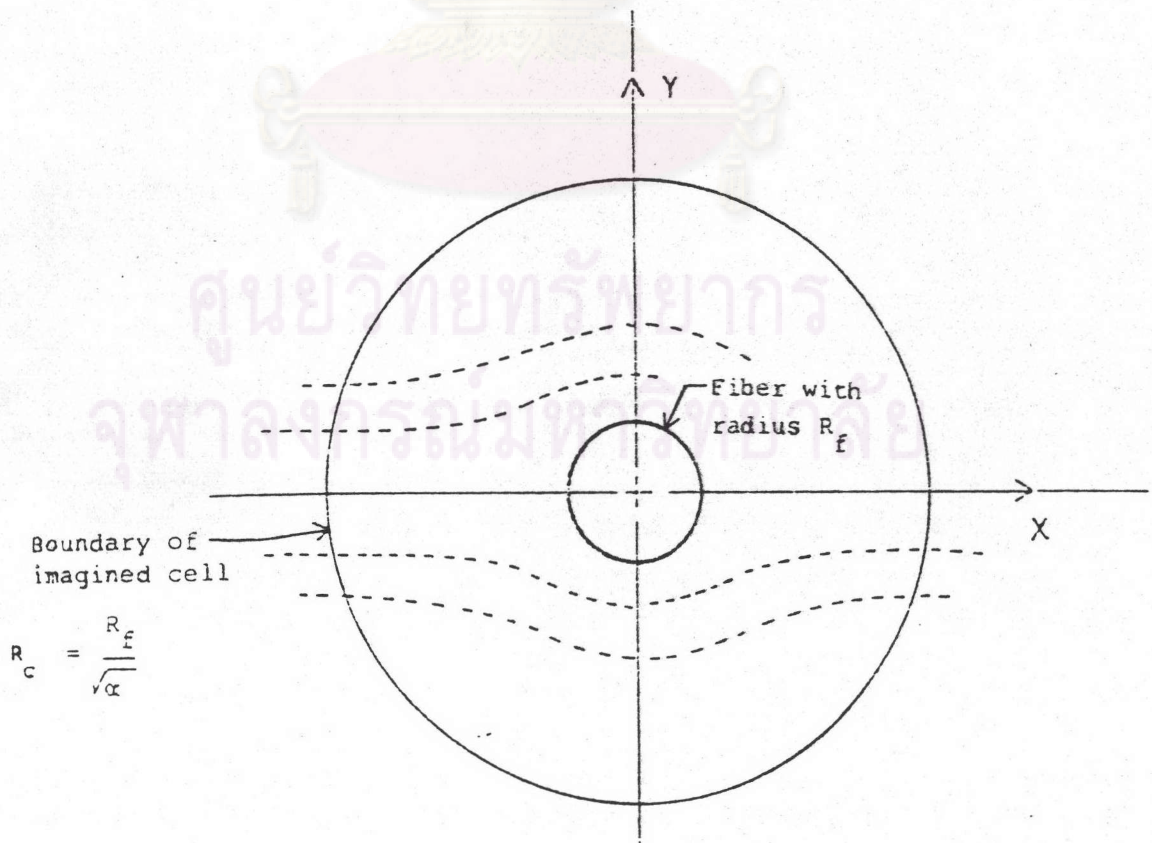

Figure 3.2 Cross section of Kuwabara's cell

$$U_x = \frac{\partial \psi}{\partial Y},\ U_y = \frac{\partial \psi}{\partial X},\ U_z = 0 \tag{3.5}$$

where $K = -\frac{1}{2}\ln\alpha + \alpha - \frac{\alpha^2}{4} - \frac{3}{4}$ and $X = \frac{x}{R_f},\ Y = \frac{y}{R_f},\ Z = \frac{z}{R_f}$

3.1.2 Single fiber; representation of a fibrous filter

A fibrous filter consists of a mass of fibers which are placed perpendicular to the direction of flow and oriented randomly. The single fiber may be used to explain the performance of a fibrous filter. The filter is thought of as a pad of thickness h at right angles to the airflow. Suppose the total length of every fiber in unit thickness of unit cross flow area is L. The packing density, α or volume fraction of the fibers is the ratio of the total volume of all the fibers to the volume of the filter. If R_f is the radius of the fiber, then

$$\alpha = \pi R_f^2 L \tag{3.6}$$

If the filter consists of fibers of length L_i and radius R_{fi}, and so on

$$\alpha = \pi R_{fi}^2 L_i \tag{3.7}$$

The definition of the dust collection efficiency of a single fibers, η, is the ratio of the distance between two the limiting streamline of the flow approaching the fiber to the fiber radius (cf. Figure 3.3).

$$\eta = \frac{Y}{R_f} \tag{3.8}$$

The change in aerosol number concentration across a fibrous mat of thickness dx is given by

$$-\frac{dn}{dx} = \frac{2n\eta L R_f}{(1-\alpha)} \tag{3.9}$$

where n is the number concentration of aerosol particles

From equation (3.6) and (3.9);

$$-\frac{dn}{n} = \frac{2\eta\alpha}{\pi(1-\alpha)R_f}dx \tag{3.10}$$

Integrating across the thickness, h, of the filter gives

$$\frac{n}{n_0} = \exp[-\frac{2h\eta\alpha}{\pi(1-\alpha)R_f}] \tag{3.11}$$

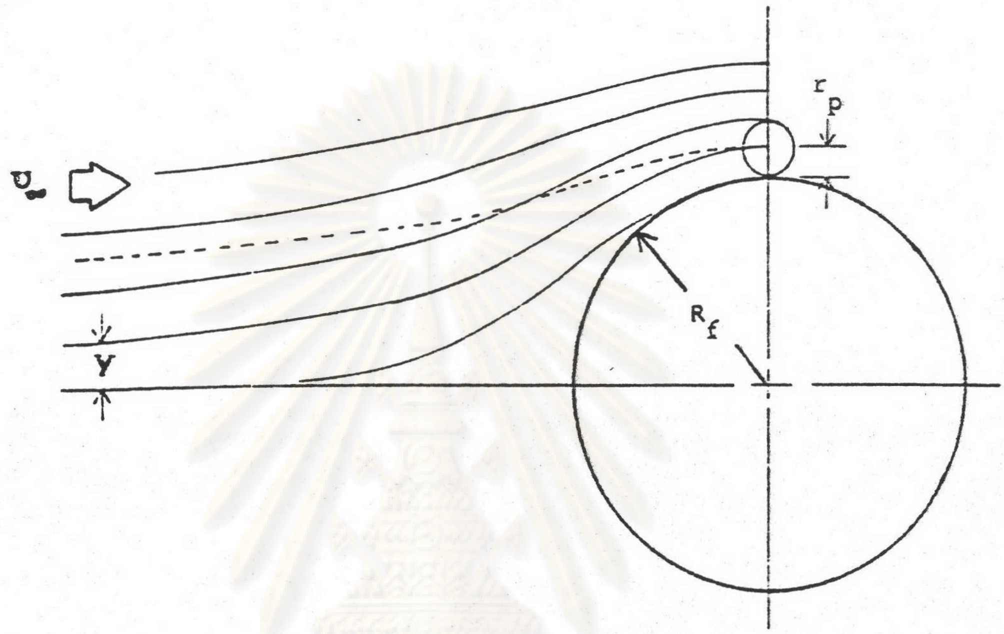

Figure 3.3 Streamlines near a cylinder fiber lying transverse to flow, and the definition of single fiber efficiency

So, the total efficiency E of the filter composed of many fibers in the mat can be related to the single fiber efficiency η as follows

$$E = 1 - \frac{n}{n_0} = 1 - \exp[-\frac{2h\eta\alpha}{\pi(1-\alpha)R_f}] \qquad (3.12)$$

The values of the single fiber efficiency which are calculated from an accurate theory of depostion of aerosol particles on a single fiber, are higher than their experimental results because the dispersion of fibers in a real filter is non-uniform, some fibers might clump together, some screen one another and not all of them lie transverse to airflow.

3.1.3 Filtration mechanism.

The filtration by a fibrous air filter depends on several mechanisms. The important mechanism causing particle deposition, are interception, diffusion, inertial impaction and gravitational settling. The single fiber efficiency η can be estimated as the sum of the individual efficiency caused by diffusion, η_D, interception, η_R,inertial impaction, η_I, and gravitational settling, η_G, mechanisms.

<u>Interception</u>

Even if a particle does not deviate from its streamline, if the distance between the particle to a capturing surface is less than the particle radius, the particle may be collected on the surface by the interception mechanism. The particle would adhere to it due to Van der Waal's force. The depostion by interception is shown in Figure 3.4c. This mechanism is directly related to the relative size of the particle. The dimensionless parameter describing the interception effect is the interception parameter R defined as the ratio of the particle diameter to the fiber diameter.

$$R = \frac{d_p}{d_f} \qquad (3.13)$$

where d_p is the particle diameter and d_f is the fiber diameter.

If the Kuwabara flow field is used, the single fiber efficiency caused by interception can be expressed by

$$\eta_R = \frac{1+R}{2K}[2\ln(1+R) - 1 + \alpha + (\frac{1}{1+R})^2(1-\frac{\alpha}{2}) - \frac{\alpha}{2}(1+R)^2] \quad (3.14)$$

Diffusion

When a particle is very small, such as the submicron order size, the main deposition mechanism is Brownian diffusion. Generally, the particle does not follow its streamline but continuously diffuses away from it. Thus the particle may be captured even on the rear surface. The depostion by diffusion is shown in Figure 3.4b. The diffusional depostion of particles increases when the particle size and air velocity decrease. From the convective diffusion equation describing this process, a dimensionless parameter called the Peclet number, Pe, can be expressed by

$$Pe = \frac{d_f U_\infty}{D_{BM}} \quad (3.15)$$

where U_∞ is the average air velocity and D_{BM} is the diffusion coefficient of the particle. The single fiber efficiency, based on Kuwabara flow field, can be expressed by (Stechkina and Fuchs, 1966)

$$\eta_D = 2.9K^{-\frac{1}{3}}Pe^{-\frac{2}{3}} + 0.624Pe^{-1} \quad (3.16)$$

$$\eta_{DR} = 1.24K^{-\frac{1}{2}}Pe^{-\frac{1}{2}}R^{\frac{2}{3}} \quad (3.17)$$

Inertial Impaction

A particle with a finite mass may not follow the streamlines exactly due to their inertia. If the streamlines are highly curved and the particle mass is high, the particle will deviate from the streamlines to collide with the capturing surface. The depostion by inertial impaction is shown in Figure 3.4a. Unlike the diffusion mechanism, the inertial impaction mechanism increases with an increase in particle size and/or air velocity. The effect of inertia on the particle can be described by the dimensionless number Stokes number, St, defined as

$$St = \frac{C_m d_p^2 \rho_p U_\infty}{9\mu d_f} \quad (3.18)$$

The single fiber efficiency is calculated by Stechkina et al. (1969), using the Kuwabara flow field. Their expression gave

$$\eta_I = \frac{1}{(2K)^2} I.St \qquad (3.19)$$

where $I = [(29.6 - 28\alpha^{0.62})R^2 - 27.5R^{2.8}]$

<u>Gravitational settling</u>

When a particle is in a gravitational force field, they will settle with a finite velocity. If the settling velocity is large, the particle may deviate from the streamlines and deposite on the capturing surface. The depostion by gravitational settling is shown in Figure 3.4d. The gravitational settling mechanism is important only for large particles and at low flow velocity. The dimensionless parameter governing the gravitational settling mechanism is

$$Gr = \frac{U_\infty}{V_g} \qquad (3.20)$$

where V_g is the settling velocity of the particle.

The single fiber efficiency due to gravity, η_G, can be approximated (Davies 1973) as

$$\eta_G = \frac{Gr}{1 + Gr} \qquad (3.21)$$

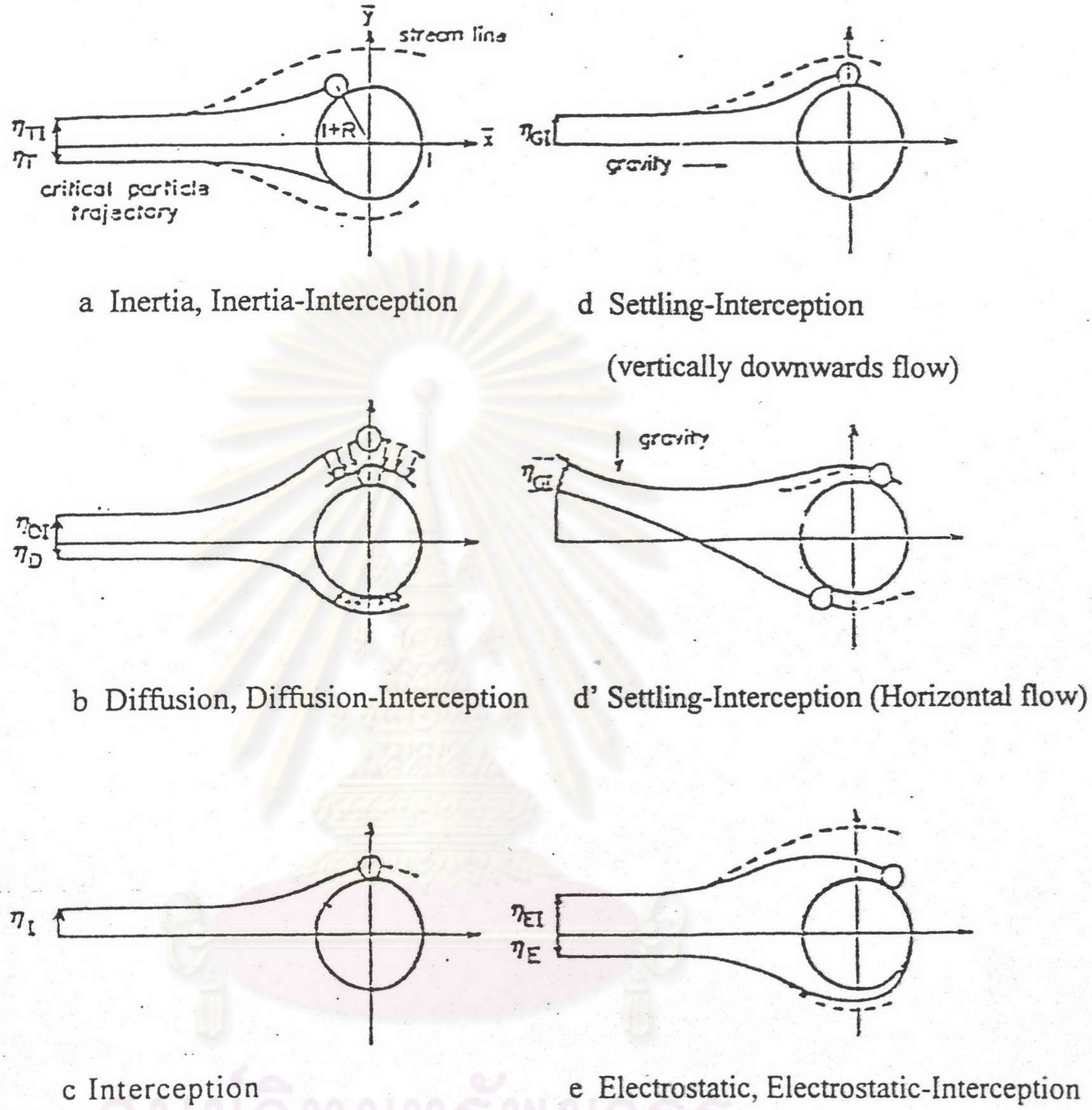

Figure 3.4 Collection mechanisms of aerosol particle

3.2 The stochastic dendritic growth model

Stochastic or random processes abound in nature such as the path of a particle in Brownian diffusional motion, the growth of population of bacteria ,and the mixing of pigment in plastics. If investigators would like to study these phenomena, they can easily make use of the theory of stochastic process.

This study extends the previous stochastic model (Kanaoka et al., 1980, 1983) which was originally a stochastic model for simulating the convective diffusional and inertial impactional deposition of the aerosols via Monte Carlo method.

To calculate the collection performance of a single fibers, the motion of the aerosol particle can be described by Kuwabara stream function, which was shown in Equaton (3.4). Figure 4.1 is a schematic diagram of a representative fiber surrounded by Kuwabara's cell. Due to its stochastic nature, the uniform random number is used to represent the random location of each incoming particle at the generation plane of Kuwabara's cell. The motion of each paritcle is governed by the Langevin's equation, as follows

$$\frac{dV}{dt} = -\frac{(V-U)}{St} + A(t) \tag{3.22}$$

where V is the velocity of the particle

U is the velocity of fluid stream

A(t) is a fluctuation force

In the case of convective diffusional depositon, the position K of a particle at time $t_i = t_{i-1} + \Delta t$ can be approximated by the following equation (3.23)

$$K_i = K_{i-1} + U_{i-1}\Delta t + 2\sqrt{\frac{\Delta t}{Pe}}n_{i-1} \tag{3.23}$$

Here, the fluid velocity U of viscous flow across a random array of parallel fibers having packing density α is given by using equation (3.5), Pe is Peclet number, and n represents the uniform random number. On the right side of equation, the second term represents the convective movement of particle, and the last term represents the diffusion movement of particle.

In the case of the inertial impactional deposition, the position of a particle at time $t_i = t_{i-1} + \Delta t$ can be approximated by the following equations (3.24) and (3.25)

$$St\frac{d^2X}{dt^2}+\frac{dX}{dt}-U_x=0 \qquad (3.24)$$

$$St\frac{d^2Y}{dt^2}+\frac{dY}{dt}-U_y=0 \qquad (3.25)$$

In short, Equations (3.23),(3.24) and (3.25) can be used to simulate the movement of a particle in Kuwabara's cell. To complete the stochastic simulation of the dendritic growth on a fiber, the following assumptions have been made.

1) Existence of dendrites on the fiber has little effect on the flow field around the fiber.

2) Spatial and time distribution of the incoming particles are random microscopically.

3) The next particle will not enter the Kuwabara's cell until the present one in it either deposits or passes through the cell.

4) A particle is always retained once it is captured on a dendrite or fiber surface.

5) There is no re-entrainment or detachment of captured particles or dendrites from the fiber.

6) The inlet particle size is uniform.

3.3 The deterministic dendritic growth model

The number and size of dendrites on a fiber surface depend not only on the filtration conditions such as fluid velocity, particle diameter, and fiber diameter, but also on the typical morphology of dendrites on a fiber. Recently, a simple deterministic model has been successfully developed (Tanthapanichakoon et al., 1993). Schematically the birth of dendrites of size 1 and the growth of dendrites of size N-1 to size N can be expressed as follows.

Birth of dendrites (size 1)

$I+SV\rightarrow P_1$

Growth of dendrites

$I+P_1\rightarrow P_2$

$I+P_2\rightarrow P_3$

:   :   :

$I+P_{N-1}\rightarrow P_N$

Here I is an incoming particle captured either on the vacant fiber surface (SV) or by an existing dendrite (P_i). The birth of dendrites, the collection of an incoming particle on a fiber surface can be considered to be proportional to the fraction of vacant surface on the fiber and the collection efficiency of the clean fiber η_0, while it will disappear and become a larger dendrite by the attachment of the next particle on it. Therefore, the net rate of birth of dendrites of size 1 is expressed by Equation (3.26).

$$\frac{dP_1}{dN_{gen}} = \eta_0[(1-S')-S_1] = \eta_0[(1-2R^2\sum_{N=1}^{\infty} Ne'_N P_N)-2R^2 e_1 P_1] \qquad (3.26)$$

Here, S1 is the effective capture area of an incoming particle by dendrite of size 1 and (1-S') is the effective vacant surface is the total fiber surface area minus the sum of the areas directly and indirectly occupied (shadowed) by the dendrites.

$$S_1 = e_1(2R^2) \qquad (3.27)$$

$$(1-S') = 1-2R^2\sum_{N=1}^{\infty} Ne'_N P_N \qquad (3.28)$$

Similary, the number of dendrites of size N increases by the depostion of one particle on the dendrites of size (N-1) but decreases by the deposition of one more particle on the dendrites of itself. Therefore, the net rate of growth of dendrites of size N (N=2,3,4,...) is expressed by Equation (3.29).

$$\frac{dP_N}{dN_{gen}} = \eta_0(S_{N-1}-S_N) = \eta_0[2R^2((N-1)e_{N-1}P_{N-1}-Ne_N P_N)] \qquad (3.29)$$

Here S_{N-1} and S_N are the effective capture area of an incoming particle by the dendrite of size N-1 and N

$$S_N = e_N(2NR^2) \qquad (3.30)$$

Furthermore, total number of dendrite of all size P_{tol}, total captured particles N_{cap} and average size of dendrite $Size_{av}$are given respectively by

$$P_{tol} = \sum_{N=1}^{\infty} P_N \qquad (3.31)$$

$$N_{cap} = \sum_{N=1}^{\infty} NP_N \qquad (3.32)$$

$$Size_{av} = \frac{N_{cap}}{P_{tol}} \qquad (3.33)$$

Initial conditions: At Ngen=0 , $P_1=P_2=P_3=...=P_N=0$

The collection efficiency of a dust-loaded fiber η is theoretically given by

$$\frac{\eta}{\eta_0} = 1 + 2R^2 \sum_{N=1}^{\infty} NP_N (e_N - e'_N) \tag{3.34}$$

According to several previous studies (Yoshioka et al., 1969; Kanaoka et al. 1980,1983), it can also be approximated by

$$\frac{\eta}{\eta_0} = 1 + \lambda m \tag{3.35}$$

where λ is the collection efficiency raising factor, and m (kg/m^3 filter) is the dust load. Here

$$m = \frac{4}{3} \rho_P \alpha R^3 \sum_{N=1}^{\infty} NP_N \tag{3.36}$$

In other words, λ is theoretically related to e_N and e'_N by

$$\lambda = \frac{3 \sum_{N=1}^{\infty} (e_N - e'_N) NP_N}{2 \rho_P R \alpha \sum_{N=1}^{\infty} NP_N} \tag{3.37}$$

For simplicity, it will be assumed that the parameters e_N and e'_N are independent of time and the dendrite size. Then

$$\lambda = \frac{3(e_N - e'_N)}{2 \rho_P R \alpha} \tag{3.38}$$

To complete the deterministic simulation of dendritic growth on a single fiber, the following assumptions have been made.

1) There is no re-entrainment of deposited particles.

2) There is no cross-linking or bridging of dendrites.

3) The incoming particle size is uniform.